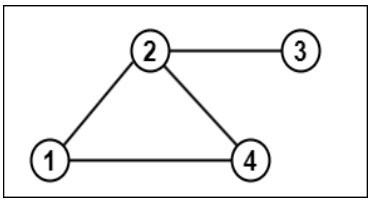
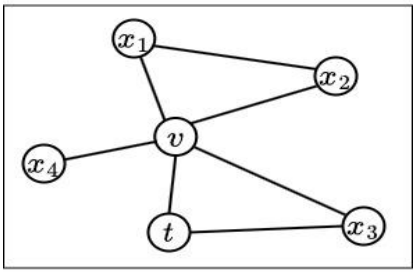
Mid-term Exam (Graph Neural Networks –Fall 2023)

Full Name:
Student ID:

1. Consider an undirected graph G of four nodes given in the following figure. The normalized adjacency matrix is defined as: $\tilde{A} = D^{-1} \cdot A$, where A is the adjacency matrix of G and D is the node degree matrix.
   a) Calculate the matrix $\tilde{A}$
   b) Calculate the 2-step transition probability matrix $\tilde{A}^2$



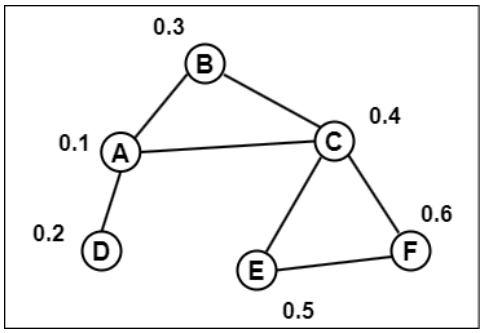
2. Consider the Node2vec algorithm with the return parameter $p = 0.2$ and the in-out parameter $q = 0.6$. A walker traversed from node t to node v and now resides at node v. Calculate the transition probabilities from node v to other nodes.



3. Consider an undirected graph G of six nodes A, B, C, D, E, and F given in the following figure. Each node has initial features that are the numbers standing next to it (i.e., the initial feature of node 'A' is $X_A^{(0)} = 0.1$). Assume that the feature of a node i at layer k can be updated as:

$$X_i^{(k)} = F\left(X_i^{(k-1)}, N_i^{(k-1)}\right),$$

   where $F(\bullet)$ returns a numeric value that is the mean (average) of its arguments, $N_i^{(k-1)}$ is the set of features of the neighbours of node i at layer $(k-1)$.
   a) Calculate the feature of each node at $k = 1$.
   b) Calculate the feature of each node at $k = 2$.



4. Given a graph with an adjacency matrix A and initial node feature matrix $H^{(0)}$ as follows:

$$A = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix} \qquad H^{(0)} = \begin{bmatrix} 0 & 0 \\ 1 & -1 \\ 2 & -2 \\ 3 & -3 \\ 4 & -4 \\ 5 & -5 \end{bmatrix}$$

Assume that the hidden layer of an GCN model of all nodes at layer (k) can be calculated as:

$$H^{(k)} = \sigma\left(A \cdot H^{(k-1)}\right),$$

where $H^{(k)}$ denotes the output at layer k, σ is a ReLU function $\mathrm{ReLU}(x) = \max(0, x)$. Calculate the output of the GCN model at layer $k = 1$.